

DICTATOR FUNCTIONS MAXIMIZE MUTUAL INFORMATION

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Let (\mathbf{X}, \mathbf{Y}) denote n independent, identically distributed copies of two arbitrarily correlated Rademacher random variables (X, Y) on $\{-1, 1\}$. We prove that the inequality $I(f(\mathbf{X}); g(\mathbf{Y})) \leq I(X; Y)$ holds for any two Boolean functions: $f, g: \{-1, 1\}^n \rightarrow \{-1, 1\}$ ($I(\cdot; \cdot)$ denotes mutual information.) We further show that equality in general is achieved only by the dictator functions: $f(\mathbf{x}) = \pm g(\mathbf{x}) = \pm x_i$ for every $i \in \{1, 2, \dots, n\}$.

1. Introduction and Main Results. Boolean functions are an important tool e.g. in complexity theory, digital circuit design, and cryptography [10]. Furthermore, they are the basis of an efficient data structure known as zero-suppressed binary decision diagram. In this paper, we study how well Boolean functions preserve the mutual information between two correlated binary sources. More specifically, let (X, Y) be two dependent Rademacher random variables on $\{-1, 1\}$, i.e., their expectation is $\mathbb{E}[X] = \mathbb{E}[Y] = 0$. By defining the correlation $\rho := \mathbb{E}[XY] \in [-1, 1]$, the mutual information [4, Section 2.3] of X and Y (in bits) equals $I(X; Y) = 1 - h_0(r)$, where $r := \mathbb{P}\{X = Y\} = \frac{1}{2}(1 + \rho) \in [0, 1]$ and $h_0(r) := -r \log_2(r) - (1 - r) \log_2(1 - r)$ is the binary entropy function. For given $n \in \mathbb{N}$, let (\mathbf{X}, \mathbf{Y}) be n independent, identically distributed copies of (X, Y) . Motivated by problems in computational biology [8], Kumar and Courtade formulated the following conjecture [9].

CONJECTURE 1. *For any Boolean function $f: \{-1, 1\}^n \rightarrow \{-1, 1\}$,*

$$(1) \quad I(f(\mathbf{X}); \mathbf{Y}) \leq 1 - h_0(r).$$

Conjecture 1 appears to be innocent at first sight and indeed it is trivial to see that any of the dictator functions [10, Definition 2.3] $f(\mathbf{x}) = x_i$, $i \in \{1, 2, \dots, n\}$, achieves equality. However, the conjecture turns out to be much more involved and cannot be established by standard information-theoretic

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arguments or by induction over n . Furthermore, Conjecture 1 can hold only for Rademacher random variables, i.e., a generalization to arbitrary binary sources is impossible [2, Section I.A]. Conjecture 1 has received significant interest and several efforts were made to find a proof (see the discussion in [3, Section IV]). Recently, Ordentlich et al. [11] used Fourier-analytic techniques and leveraged hypercontractivity to improve upon previously known bounds for $I(f(\mathbf{X}); \mathbf{Y})$. Kindler et al. [7] studied an analogous problem in Gaussian spaces.

We next state the main result of this paper, which is a relaxed version of Conjecture 1 involving two Boolean functions.

THEOREM 1. *For any two Boolean functions $f, g: \{-1, 1\}^n \rightarrow \{-1, 1\}$,*

$$(2) \quad I(f(\mathbf{X}); g(\mathbf{Y})) \leq I(\mathbf{X}; \mathbf{Y}) = 1 - h_0(r).$$

Assuming that (1) is true, this statement would readily follow from the data processing inequality [4, Theorem 2.8.1]. While being weaker than Conjecture 1, it seems that standard information-theoretic tools are still insufficient for establishing Theorem 1. In fact, Theorem 1 was stated as an open problem in the original publication [9, Section IV] and in [3]. A proof of (2) was previously available only under the additional restrictive assumptions that f and g are equally biased (i.e., $\mathbb{E}[g(\mathbf{X})] = \mathbb{E}[f(\mathbf{X})]$) and satisfy the condition

$$(3) \quad \mathbb{P}\{f(\mathbf{X}) = 1, g(\mathbf{X}) = 1\} \geq \mathbb{P}\{f(\mathbf{X}) = 1\} \mathbb{P}\{g(\mathbf{X}) = 1\}.$$

See [3, Section IV] for further details.

In this paper, we use Fourier-analytic tools to prove Theorem 1 without any restrictions on f and g . More specifically, we suitably bound the Fourier coefficients of f and g and thereby reduce (2) to elementary inequalities, which subsequently are established via standard arguments. Like Conjecture 1, Theorem 1 doesn't hold for arbitrary binary asymmetric sources: using the counterexample from [2, Section I.A] it follows that our Fourier-analytic proof will not carry over to p -biased Fourier analysis [14, 15]. We note that Anantharam et al. [2] showed that Theorem 1 would follow from a conjectured result concerning the hypercontractivity ribbon of two binary random variables; however, that conjecture itself remains unproven to date.

The i -th dictator function is defined as $\chi_i: \{-1, 1\}^n \rightarrow \{-1, 1\}$, $\chi_i(\mathbf{x}) := x_i$. Evidently, the Boolean functions $f = g = \chi_i$ maximize $I(f(\mathbf{X}); g(\mathbf{Y}))$ and achieve equality in (2). A careful inspection of the proof of Theorem 1 reveals that up to sign changes the dictator functions in general are the unique maximizers of $I(f(\mathbf{X}); g(\mathbf{Y}))$. For the degenerate case $\rho = 0$ (independent sources), the upper bound $I(f(\mathbf{X}); g(\mathbf{Y})) = 0$ is trivially achieved by any

two Boolean functions f, g . Similarly, for the case $\rho = \pm 1$ (deterministically dependent sources), the upper bound $I(f(\mathbf{X}); g(\mathbf{Y})) = 1$ is achieved by any two unbiased Boolean functions f and g that satisfy $g(\mathbf{x}) = \pm f(\text{sgn}(\rho)\mathbf{x})$. The following uniqueness result is the second main contribution of the paper.

PROPOSITION 1. *For the non-degenerate case $0 < |\rho| < 1$, equality in (2) is achieved if and only if $f = \pm g = \pm \chi_i$ for some $i \in \{1, 2, \dots, n\}$.*

2. Notation and Background. We use $\mathbb{E}[\cdot]$ as the expectation operator and $\mathbb{P}\{\cdot\}$ to denote the probability of an event. Define $\Omega := \{-1, 1\}$ and let (\mathbf{X}, \mathbf{Y}) be two Rademacher random variables on Ω , i.e., $\mathbb{E}[\mathbf{X}] = \mathbb{E}[\mathbf{Y}] = 0$. Define the correlation of \mathbf{X} and \mathbf{Y} as $\rho := \mathbb{E}[\mathbf{X}\mathbf{Y}] \in [-1, 1]$ and let $r := \mathbb{P}\{\mathbf{X} = \mathbf{Y}\} = \frac{1}{2}(1 + \rho) \in [0, 1]$. Fix $n \in \mathbb{N}$ and let (\mathbf{X}, \mathbf{Y}) be n independent, identically distributed copies of (\mathbf{X}, \mathbf{Y}) .

For convenience we define $\bar{t} := 1 - t$ for $t \in \mathbb{R}$ and use the notation $[1 : n] := \{1, 2, \dots, n\}$ for $n \in \mathbb{N}$. We denote the binary and natural logarithm by $\log_2(\cdot)$ and $\log(\cdot)$, respectively. The degree of a polynomial p will be denoted by $\deg(p)$. We will require some basic concepts from information theory, in particular mutual information and entropy [4, Section 2.3], given here for the sake of completeness. We will adopt the usual convention $0 \cdot \log_2(0) := 0$.

DEFINITION 1. *Given two random variables \mathbf{X}, \mathbf{Y} on the finite probability space $\mathcal{X} \times \mathcal{Y}$, the mutual information (in bit) of \mathbf{X} and \mathbf{Y} is given by*

$$(4) \quad I(\mathbf{X}; \mathbf{Y}) := \sum_{(x,y) \in \mathcal{X} \times \mathcal{Y}} p(x,y) \log_2 \left(\frac{p(x,y)}{p(x)p(y)} \right),$$

where $p(x,y)$ is the joint probability mass function of \mathbf{X} and \mathbf{Y} ; furthermore, $p(x) := \sum_{y \in \mathcal{Y}} p(x,y)$ and $p(y) := \sum_{x \in \mathcal{X}} p(x,y)$ denote the respective marginal. The entropy of \mathbf{X} is defined as

$$(5) \quad H(\mathbf{X}) := - \sum_{x \in \mathcal{X}} p(x) \log_2(p(x)).$$

Note that mutual information and entropy only depend on the probability mass function p and are therefore unaffected by one-to-one mappings. In the special case of a binary random variable $\mathbf{X} \in \Omega$, (5) becomes $H(\mathbf{X}) = h_0(\mathbb{P}\{\mathbf{X} = 1\})$, where $h_0(t) := -t \log_2(t) - \bar{t} \log_2(\bar{t})$ is the binary entropy function, which is symmetric around $\frac{1}{2}$ (i.e., $h_0(t) = h_0(\bar{t})$), has unique maximum $h_0(\frac{1}{2}) = 1$, and is strictly decreasing on $[\frac{1}{2}, 1]$. We will further use fundamental properties of mutual information as stated in [4, Theorem 2.4.1].

We will need several Fourier-analytic properties of Boolean functions (see e.g. [10]). The inner product of two functions $f, g: \Omega^n \rightarrow \mathbb{R}$ is defined as

$$(6) \quad \langle f, g \rangle := \mathbb{E}[f(\mathbf{X})g(\mathbf{X})] = 2^{-n} \sum_{\mathbf{x} \in \Omega^n} f(\mathbf{x})g(\mathbf{x})$$

and the norm is given by $\|f\| := \sqrt{\langle f, f \rangle}$. The Fourier-Walsh transform \hat{f} of $f: \Omega^n \rightarrow \mathbb{R}$ equals [10, Proposition 1.8]

$$(7) \quad \hat{f}(S) := \langle f, \chi_S \rangle = 2^{-n} \sum_{\mathbf{x} \in \Omega^n} f(\mathbf{x})\chi_S(\mathbf{x})$$

for each $S \subseteq [1:n]$, where $\chi_S(\mathbf{x}) := \prod_{i \in S} x_i$ is the canonical base. The special case where S is a singleton (i.e., $S = \{i\}$) leads to the dictator functions $\chi_i(\mathbf{x}) := \chi_{\{i\}}(\mathbf{x}) = x_i$, $i \in [1:n]$ [10, Definition 2.3]. Let T_ρ denote the so-called noise operator [10, Definition 2.46], defined for any function $f: \Omega^n \rightarrow \mathbb{R}$ as

$$(8) \quad T_\rho f: \Omega^n \rightarrow \mathbb{R}$$

$$(9) \quad \mathbf{x} \mapsto \mathbb{E}[f(\mathbf{Y}) | \mathbf{X} = \mathbf{x}],$$

We use the abbreviations $\alpha := \mathbb{E}[f(\mathbf{X})] = \hat{f}(\emptyset)$, $\beta := \mathbb{E}[g(\mathbf{X})] = \hat{g}(\emptyset)$, $a := \frac{1}{2}(1 + \alpha) = \mathbb{P}\{f(\mathbf{X}) = 1\}$, and $b := \frac{1}{2}(1 + \beta) = \mathbb{P}\{g(\mathbf{X}) = 1\}$. We refer to α as the bias of f and say that f is unbiased if $\alpha = 0$; similarly, g is unbiased if $\beta = 0$.

LEMMA 1. *For any two functions $f, g: \Omega^n \rightarrow \Omega$, the following properties hold for all $S \subseteq [1:n]$ and $\mathbf{x} \in \Omega^n$:*

$$(10) \quad f(\mathbf{x}) = \sum_{S \subseteq [1:n]} \hat{f}(S)\chi_S(\mathbf{x}),$$

$$(11) \quad \sum_{S \subseteq [1:n]} \hat{f}(S)^2 = 1,$$

$$(12) \quad \widehat{T_\rho f}(S) = \rho^{|S|} \hat{f}(S),$$

$$(13) \quad \langle f, g \rangle = \sum_{S \subseteq [1:n]} \hat{f}(S)\hat{g}(S) = 1 - 2\mathbb{P}\{f(\mathbf{X}) \neq g(\mathbf{X})\}.$$

The proofs of these well known properties of Boolean functions can be found, e.g., in [10, Sections 1, 2].

We use the convention that the sign of zero equals one and denote (higher-order) derivatives by (multiple) superscript primes. The notation $\pm x$ is used as a shorthand for “either $+x$ or $-x$.”

3. Proof of Theorem 1. We first argue that due to the invariances of mutual information and the symmetry of the binary entropy function, it suffices to prove Theorem 1 for $\rho \geq 0$ and $\beta \geq \alpha \geq 0$ (recall that $\alpha = \hat{f}(\emptyset)$, $\beta = \hat{g}(\emptyset)$). Note that $\beta \geq \alpha \geq 0$ is equivalent to $\frac{1}{2} \leq a \leq b$.

For n i.i.d. random variables (\mathbf{X}, \mathbf{Y}) with arbitrary correlation $\rho = 2r - 1$, define $\tilde{\mathbf{Y}} := \text{sgn}(\rho)\mathbf{Y}$ such that the correlation of the i.i.d. variables $(\mathbf{X}, \tilde{\mathbf{Y}})$ equals $\tilde{\rho} = |\rho|$; correspondingly, $\tilde{r} := (1 + \tilde{\rho})/2 = (1 + |\rho|)/2 = \max\{r, 1 - r\}$. Furthermore, for arbitrary Boolean functions $f(\mathbf{x})$ and $g(\mathbf{y})$ define

$$(14) \quad f^{(0)}(\mathbf{x}) := \text{sgn}(\alpha)f(\mathbf{x}),$$

$$(15) \quad g^{(0)}(\mathbf{y}) := \text{sgn}(\beta)g(\mathbf{y}),$$

$$(16) \quad g^{(1)}(\tilde{\mathbf{y}}) := g^{(0)}(\text{sgn}(\rho)\tilde{\mathbf{y}}) = g^{(0)}(\mathbf{y}).$$

We have $\hat{f}^{(0)}(\emptyset) = |\alpha| \geq 0$ and $\hat{g}^{(0)}(\emptyset) = \hat{g}^{(1)}(\emptyset) = |\beta| \geq 0$. Since mutual information is invariant to one-to-one mappings, it follows that $I(f(\mathbf{X}); g(\mathbf{Y})) = I(f^{(0)}(\mathbf{X}); g^{(0)}(\mathbf{Y})) = I(f^{(0)}(\mathbf{X}); g^{(1)}(\tilde{\mathbf{Y}}))$. We may assume without loss of generality that $|\alpha| \leq |\beta|$; otherwise, we swap f and g without affecting mutual information. Assuming that Theorem 1 holds for $|\rho| \geq 0$ and $|\beta| \geq |\alpha|$, it follows that

$$(17) \quad I(f(\mathbf{X}); g(\mathbf{Y})) = I(f^{(0)}(\mathbf{X}); g^{(1)}(\tilde{\mathbf{Y}}))$$

$$(18) \quad \leq 1 - h_0(\tilde{r})$$

$$(19) \quad = 1 - h_0(r),$$

where in the last step we used the symmetry $h_0(r) = h_0(1 - r)$ of the binary entropy function. This confirms that if Theorem 1 holds for nonnegative ρ and $\beta \geq \alpha \geq 0$, it actually holds for arbitrary ρ , α , and β .

3.1. Auxiliary Results. Before proving Theorem 1 for nonnegative ρ and $\beta \geq \alpha \geq 0$, we need to establish a few auxiliary results.

LEMMA 2. *For any $\rho \in [-1, 1]$ the following bounds hold:*

$$(20) \quad \alpha + \beta - 1 \leq \langle f, T_\rho g \rangle \leq 1 + \alpha - \beta$$

PROOF. As $f - 1 \leq 0$, $f + 1 \geq 0$, and $g - 1 \leq 0$, we obtain the desired bounds

$$(21) \quad 0 \leq \langle f - 1, T_\rho(g - 1) \rangle = \langle f, T_\rho g \rangle - \alpha - \beta + 1,$$

$$(22) \quad 0 \geq \langle f + 1, T_\rho(g - 1) \rangle = \langle f, T_\rho g \rangle - \alpha + \beta - 1.$$

□

The following lemma formalizes the minimization and maximization of a twice differentiable real-valued convex function on a compact interval. It follows from Taylor's Theorem [12, Theorem 5.15] and [12, Theorem 5.8].

LEMMA 3. *Consider a function $\phi: I \rightarrow \mathbb{R}$ defined on the compact interval $I := [t_1, t_2] \subset \mathbb{R}$ with $t_1 < t_2$. If the first-order derivative ϕ' is continuous on I and the second-order derivative $\phi''(t)$ exists for every $t \in I^\circ := (t_1, t_2)$, then the following two properties hold:*

1. *If $\phi''(t) \geq 0$ for all $t \in I^\circ$, and $\phi'(t^*) = 0$ for some $t^* \in I$, then $\phi(t) \geq \phi(t^*)$ for all $t \in I$. Furthermore, if $\phi''(t) > 0$ for all $t \in I^\circ$, and $\phi'(t^*) = 0$ for some $t^* \in I$, then $\phi(t) > \phi(t^*)$ for all $t \in I \setminus \{t^*\}$.*
2. *If $\phi''(t) \leq 0$ for all $t \in I^\circ$, then $\phi(t) \geq \min\{\phi(t_1), \phi(t_2)\}$ for all $t \in I$. Furthermore, if $\phi''(t) < 0$ for all $t \in I^\circ$, then $\phi(t) > \min\{\phi(t_1), \phi(t_2)\}$ for all $t \in I^\circ$.*

We will furthermore need the following powerful lemma, which allows us to obtain the necessary bounds on the parameters of the joint distribution of $f(\mathbf{X})$ and $g(\mathbf{Y})$. We define two sets of index sets for which the Fourier transforms of $f(\mathbf{X})$ and $g(\mathbf{Y})$ are both non-zero and have identical and opposite signs, respectively, i.e., $\mathcal{P} := \{S \subseteq [1:n] : \hat{f}(S)\hat{g}(S) > 0\} \setminus \{\emptyset\}$ and $\mathcal{N} := \{S \subseteq [1:n] : \hat{f}(S)\hat{g}(S) < 0\}$. We further recall that $\alpha = \mathbb{E}[f(\mathbf{X})] = \hat{f}(\emptyset)$, $\beta = \mathbb{E}[g(\mathbf{X})] = \hat{g}(\emptyset)$, $a = \frac{1}{2}(1 + \alpha) = \mathbb{P}\{f(\mathbf{X}) = 1\}$, $b = \frac{1}{2}(1 + \beta) = \mathbb{P}\{g(\mathbf{X}) = 1\}$, and that an overbar denotes the complement $\bar{t} = 1 - t$.

LEMMA 4. *The Fourier transforms of any two Boolean functions $f, g: \Omega^n \rightarrow \Omega$ with $\beta \geq \alpha \geq 0$ satisfy*

$$(23) \quad \sum_{S \in \mathcal{P}} \hat{f}(S)\hat{g}(S) \leq 2\left(a\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right),$$

$$(24) \quad \sum_{S \in \mathcal{N}} \hat{f}(S)\hat{g}(S) \geq -2\left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right).$$

For $\alpha = \beta = 0$, equality in (23) or (24) can only hold if $g = \pm f$.

PROOF. We show the inequalities

$$(25) \quad \sum_{S \in \mathcal{P}} \hat{f}(S)\hat{g}(S) - \sum_{S \in \mathcal{N}} \hat{f}(S)\hat{g}(S) \leq 4\sqrt{a\bar{a}b\bar{b}},$$

$$(26) \quad \sum_{S \in \mathcal{P}} \hat{f}(S)\hat{g}(S) + \sum_{S \in \mathcal{N}} \hat{f}(S)\hat{g}(S) \geq -4\bar{a}\bar{b},$$

$$(27) \quad \sum_{S \in \mathcal{P}} \hat{f}(S) \hat{g}(S) + \sum_{S \in \mathcal{N}} \hat{f}(S) \hat{g}(S) \leq 4a\bar{b}.$$

The upper bound (23) can be obtained by adding (25) and (27) and the lower bound (24) follows by subtracting (25) from (26).

Subtracting the means of f and g yields the unbiased functions $f_0 := f - \alpha$, $g_0 := g - \beta$. We then define f_1 and g_1 in terms of their Fourier transforms $\hat{f}_1(S) := |\hat{f}_0(S)|$ and $\hat{g}_1(S) := |\hat{g}_0(S)|$. With these definitions, (25) is obtained as

$$\begin{aligned} (28) \quad \sum_{S \in \mathcal{P}} \hat{f}(S) \hat{g}(S) - \sum_{S \in \mathcal{N}} \hat{f}(S) \hat{g}(S) &= \sum_{S \subseteq [1:n]} |\hat{f}_0(S)| |\hat{g}_0(S)| \\ (29) \quad &= \langle f_1, g_1 \rangle \\ (30) \quad &\leq \|f_1\| \|g_1\| \\ (31) \quad &= \sqrt{(1 - \alpha^2)(1 - \beta^2)} \\ (32) \quad &= 4\sqrt{a\bar{a}b\bar{b}}, \end{aligned}$$

where (30) follows from the Cauchy-Schwarz inequality [13, 4.2]. To show (26) and (27), note that

$$\begin{aligned} (33) \quad \sum_{S \in \mathcal{P}} \hat{f}(S) \hat{g}(S) + \sum_{S \in \mathcal{N}} \hat{f}(S) \hat{g}(S) &= \sum_{S \subseteq [1:n]} \hat{f}_0(S) \hat{g}_0(S) \\ (34) \quad &= \langle f_0, g_0 \rangle \\ (35) \quad &= \langle f, g \rangle - \alpha\beta. \end{aligned}$$

The bounds $\alpha + \beta - 1 \leq \langle f, g \rangle \leq 1 + \alpha - \beta$ follow from Lemma 2 with $\rho = 1$. We obtain (26) by substituting in (35),

$$\begin{aligned} (36) \quad \langle f_0, g_0 \rangle &= \langle f, g \rangle - \alpha\beta \\ (37) \quad &\geq \alpha + \beta - 1 - \alpha\beta \\ (38) \quad &= -(1 - \alpha)(1 - \beta) \\ (39) \quad &= -4\bar{a}\bar{b}. \end{aligned}$$

Similarly, we obtain (27) by noticing:

$$\begin{aligned} (40) \quad \langle f_0, g_0 \rangle &\leq 1 + \alpha - \beta - \alpha\beta \\ (41) \quad &= (1 + \alpha)(1 - \beta) \\ (42) \quad &= 4a\bar{b} \end{aligned}$$

To show the necessary condition for equality in (24), assume $\alpha = \beta = 0$ and define $W_P := \sum_{S \in \mathcal{P}} \hat{f}(S)^2$ and $W_N := \sum_{S \in \mathcal{N}} \hat{f}(S)^2$. Due to (11) we

have $W_P + W_N = 1$. Equality in either (24) or (23) necessitates equality in (30). The Cauchy-Schwarz inequality is satisfied with equality only if $g_1 = \lambda f_1$ for some $\lambda \in \mathbb{R}$. Since $\hat{f}_1(S)$ and $\hat{g}_1(S)$ are both nonnegative for all $S \subseteq [1:n]$ and have unit norm, necessarily $\lambda = 1$. We further have

$$(43) \quad g(\mathbf{x}) = \sum_{S \subseteq [1:n]} \hat{g}(S) \chi_S(\mathbf{x})$$

$$(44) \quad = \sum_{S \in \mathcal{P} \cup \mathcal{N}} \text{sgn}(\hat{g}(S)) \hat{g}_1(S) \chi_S(\mathbf{x})$$

$$(45) \quad = \sum_{S \in \mathcal{P} \cup \mathcal{N}} \text{sgn}(\hat{g}(S)) \hat{f}_1(S) \chi_S(\mathbf{x})$$

$$(46) \quad = \sum_{S \in \mathcal{P} \cup \mathcal{N}} \text{sgn}(\hat{g}(S) \hat{f}(S)) \hat{f}(S) \chi_S(\mathbf{x})$$

$$(47) \quad = \sum_{S \in \mathcal{P}} \hat{f}(S) \chi_S(\mathbf{x}) - \sum_{S \in \mathcal{N}} \hat{f}(S) \chi_S(\mathbf{x}),$$

which leads to

$$(48) \quad \langle f, g \rangle = W_P - W_N = 1 - 2W_N.$$

For equality in (24) we also need equality in (37), which is equivalent to $\langle f, g \rangle = -1$. In view of (48), this entails $W_N = 1$ and consequently $g = -f$ by (47). When requiring equality in (23), one obtains the necessary condition $g = f$ in the same manner, using equality in (40). \square

The function defined next is crucial for the proof of our main result.

DEFINITION 2. For $\frac{1}{2} \leq a \leq b < 1$ and $t \in [1 - 2(\bar{b} + \bar{a}), 1 - 2(b - a)]$ define the function

$$(49) \quad \phi_{a,b}(t) := b \log_2 \left(\frac{1}{4b} (2a + 2b - \bar{t}) \right) + \bar{b} \log_2 \left(\frac{1}{4\bar{b}} (2\bar{a} + 2\bar{b} - \bar{t}) \right).$$

We first show that $\phi_{a,b}(t)$ is strictly concave.

LEMMA 5. For $\frac{1}{2} \leq a \leq b < 1$ and $1 - 2(\bar{b} + \bar{a}) < t < 1 - 2(b - a)$, we have $\phi''_{a,b}(t) < 0$.

PROOF. We calculate the first-order derivative

$$(50) \quad \phi'_{a,b}(t) = \frac{1}{4} \log_2 \left(\frac{(2(b - a) + \bar{t})(2(\bar{b} - \bar{a}) + \bar{t})}{(2(b + a) - \bar{t})(2(\bar{b} + \bar{a}) - \bar{t})} \right)$$

and the second-order derivative

$$(51) \quad \phi''_{a,b}(t) = -\frac{1}{4\log(2)} \left(\frac{1}{2(b-a) + \bar{t}} + \frac{1}{2(\bar{b}-\bar{a}) + \bar{t}} + \frac{1}{2(b+a) - \bar{t}} + \frac{1}{2(\bar{b}+\bar{a}) - \bar{t}} \right).$$

The proof is concluded by observing that for $\frac{1}{2} \leq a \leq b < 1$ and $2(b-a) < \bar{t} < 2(\bar{b}+\bar{a})$ all terms within the parentheses in (51) are strictly positive. \square

The following result on $\phi_{a,b}(t)$ follows from elementary results in real analysis. Although conceptually simple, the proof is rather lengthy and therefore deferred to Appendix A.

LEMMA 6. For $\frac{1}{2} \leq a \leq b < 1$ and $0 \leq \rho \leq 1$, let

$$(52) \quad t_0 := \max \left\{ 1 - 2(\bar{a} + \bar{b}), 1 - 2 \left(a\bar{b} + b\bar{a} + \rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right) \right\},$$

$$(53) \quad t_1 := \min \left\{ 1 - 2(b-a), 1 - 2 \left(a\bar{b} + b\bar{a} - \rho \left(a\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right) \right\}.$$

Then,

$$(54) \quad h_0(a) - \phi_{a,b}(t_0) \leq 1 - h_0\left(\frac{1+\rho}{2}\right),$$

$$(55) \quad h_0(a) - \phi_{a,b}(t_1) \leq 1 - h_0\left(\frac{1+\rho}{2}\right),$$

with equality if and only if either $\rho = 0$ or $a = b = \frac{1}{2}$.

3.2. *Proof of Theorem 1 for $\rho \geq 0$ and $\beta \geq \alpha \geq 0$.* Since $b = 1$ entails $g \equiv 1$ and therefore $I(f(\mathbf{X}); g(\mathbf{Y})) = 0 \leq 1 - h_0(r)$, we can assume $b < 1$ in the following (in addition to $\frac{1}{2} \leq a \leq b$). We can then rewrite the mutual information of $f(\mathbf{X})$ and $g(\mathbf{Y})$ as (cf. [4, Theorem 2.4.1]):

$$(56) \quad I(f(\mathbf{X}); g(\mathbf{Y})) = H(f(\mathbf{X})) - H(f(\mathbf{X})|g(\mathbf{Y}))$$

$$(57) \quad = H(f(\mathbf{X})) - \sum_{z \in \Omega} P\{g(\mathbf{Y}) = z\} H(f(\mathbf{X})|g(\mathbf{Y}) = z)$$

$$(58) \quad = h_0(a) - b H(f(\mathbf{X})|g(\mathbf{Y}) = 1) - \bar{b} H(f(\mathbf{X})|g(\mathbf{Y}) = -1)$$

$$(59) \quad = h_0(a) - b h_0(p^+) - \bar{b} h_0(p^-),$$

with $p^+ := P\{f(\mathbf{X}) = 1|g(\mathbf{Y}) = 1\}$ and $p^- := P\{f(\mathbf{X}) = -1|g(\mathbf{Y}) = -1\}$. By deriving suitable bounds for p^+ and p^- and using (59), we will reduce (2) to elementary inequalities.

In analogy to [10, Proposition 1.9] we have

$$(60) \quad \langle f, T_\rho g \rangle = 2\mathbb{P}\{f(\mathbf{X}) = g(\mathbf{Y})\} - 1 = 1 - 2\mathbb{P}\{f(\mathbf{X}) \neq g(\mathbf{Y})\}.$$

For any two binary random variables (A, B) on Ω^2 it can be verified, that

$$(61) \quad \begin{aligned} & \mathbb{P}\{A = 1, B = 1\} \\ &= \frac{1}{2}(\mathbb{P}\{A = 1\} + \mathbb{P}\{B = 1\} + \mathbb{P}\{A = B\} - 1). \end{aligned}$$

Using (60) and (61), we obtain

$$(62) \quad p^+ = \frac{\mathbb{P}\{f(\mathbf{X}) = 1, g(\mathbf{Y}) = 1\}}{\mathbb{P}\{g(\mathbf{Y}) = 1\}}$$

$$(63) \quad = \frac{1}{2b}(\mathbb{P}\{f(\mathbf{X}) = 1\} + \mathbb{P}\{g(\mathbf{Y}) = 1\} - \mathbb{P}\{f(\mathbf{X}) \neq g(\mathbf{Y})\})$$

$$(64) \quad = \frac{1}{4b}(2a + 2b - (1 - \langle f, T_\rho g \rangle)).$$

Similarly, we have

$$(65) \quad p^- = \frac{1}{4\bar{b}}(2\bar{a} + 2\bar{b} - (1 - \langle f, T_\rho g \rangle)).$$

By using (64) and (65), we can rewrite (59) as (cf. (49)):

$$(66) \quad I(f(\mathbf{X}); g(\mathbf{Y})) = h_0(a) - \phi_{a,b}(\langle f, T_\rho g \rangle).$$

Note that by Lemma 2,

$$(67) \quad \langle f, T_\rho g \rangle \in [1 - 2(\bar{a} + \bar{b}), 1 - 2(b - a)].$$

Using (12) and (13), the bilinear form $\langle f, T_\rho g \rangle$ can be bounded as:

$$(68) \quad \langle f, T_\rho g \rangle = \sum_{S \subseteq [1:n]} \rho^{|S|} \hat{f}(S) \hat{g}(S)$$

$$(69) \quad = \alpha\beta + \sum_{S \in \mathcal{P}} \rho^{|S|} \hat{f}(S) \hat{g}(S) + \sum_{S \in \mathcal{N}} \rho^{|S|} \hat{f}(S) \hat{g}(S)$$

$$(70) \quad \geq \alpha\beta + \sum_{S \in \mathcal{N}} \rho^{|S|} \hat{f}(S) \hat{g}(S)$$

$$(71) \quad = \alpha\beta + \rho \sum_{S \in \mathcal{N}} \rho^{|S|-1} \hat{f}(S) \hat{g}(S),$$

where we used $\rho \geq 0$ and $\hat{f}(S)\hat{g}(S) \geq 0$ for $S \in \mathcal{P}$. Since $\emptyset \notin \mathcal{N}$, $\rho \in [0, 1]$, and $\hat{f}(S)\hat{g}(S) \leq 0$ for $S \in \mathcal{N}$, the bound can be further developed as:

$$(72) \quad \langle f, T_\rho g \rangle \geq \alpha\beta + \rho \sum_{S \in \mathcal{N}} \hat{f}(S)\hat{g}(S)$$

$$(73) \quad \geq \alpha\beta - 2\rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right)$$

$$(74) \quad = (2a - 1)(2b - 1) - 2\rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right)$$

$$(75) \quad = 1 - 2 \left(\bar{a}\bar{b} + b\bar{a} + \rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right).$$

where we applied Lemma 4 to obtain (73). Applying Lemma 4, we also obtain the upper bound

$$(76) \quad \langle f, T_\rho g \rangle = \alpha\beta + \sum_{S \in \mathcal{P}} \rho^{|S|} \hat{f}(S)\hat{g}(S) + \sum_{S \in \mathcal{N}} \rho^{|S|} \hat{f}(S)\hat{g}(S)$$

$$(77) \quad \leq \alpha\beta + 2\rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right)$$

$$(78) \quad = 1 - 2 \left(\bar{a}\bar{b} + b\bar{a} - \rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right).$$

In total, (67), (75) and (78) yield $t_0 \leq \langle f, T_\rho g \rangle \leq t_1$ with t_0 and t_1 as defined in Lemma 6. Invoking Lemma 5 and part 2 of Lemma 3, we obtain

$$(79) \quad I(f(\mathbf{X}); g(\mathbf{Y})) = h_0(a) - \phi_{a,b}(\langle f, T_\rho g \rangle)$$

$$(80) \quad \leq h_0(a) - \min_{t \in \{t_0, t_1\}} \phi_{a,b}(t)$$

$$(81) \quad \leq 1 - h_0(r),$$

where the last step follows from Lemma 6 and concludes the proof.

REMARK 1. There is a rich literature on the noise sensitivity of Boolean functions (see [5] for an introduction). An important concept in this area is hypercontractivity, which has also been applied in information theory [1]. Among other important results, a small-set expansion theorem was proved using hypercontractivity by Kahn, Kalai, and Linial in their landmark paper [6]. A two-set generalization of this small-set expansion theorem [10, Section 10.1] can be used to obtain bounds on $\langle f, T_\rho g \rangle$. These bounds, however, are not strong enough for proving Theorem 1 because the small-set expansion theorem is only asymptotically sharp for very biased functions. By contrast, the critical regime for (2) is in the vicinity of unbiased functions.

4. Proof of Proposition 1. Like with Theorem 1, we first show that it suffices to prove Proposition 1 for $0 < \rho < 1$. Indeed, assume $-1 < \rho < 0$. The sufficiency of $f = \pm g = \pm \chi_i$ for any $i \in [1:n]$ to achieve equality in Theorem 1 here follows immediately from

$$(82) \quad I(f(\mathbf{X}); g(\mathbf{Y})) = I(\pm \chi_i(\mathbf{X}); \pm \chi_i(\mathbf{Y})) = I(\mathbf{X}; \mathbf{Y}) = 1 - h_0(r).$$

That $f = \pm g = \pm \chi_i$ for some $i \in [1:n]$ is also necessary for equality in (2) in the case $-1 < \rho < 0$ follows from the observation that Proposition 1 for $0 < \rho < 1$ implies $f^{(0)} = \pm \chi_i$ and $g^{(1)} = \pm \chi_i$ for some $i \in [1:n]$, where we used the definitions (14) to (16). Clearly this entails $f = f^{(0)} = \pm \chi_i$ and $g(\mathbf{y}) = g^{(1)}(-\mathbf{y}) = \pm \chi_i$.

We next prove Proposition 1 for $0 < \rho < 1$. Clearly, $f = \pm g = \pm \chi_i$ for some $i \in [1:n]$ is a sufficient condition to maximize $I(f(\mathbf{X}); g(\mathbf{Y}))$. A careful inspection of the proof of Theorem 1 shows that this condition is also necessary. For equality in Theorem 1 it is necessary to obtain equality in (81), which implies $a = b = \frac{1}{2}$ by Lemma 6. This entails $t_0 = -\rho$ and $t_1 = \rho$. For equality in (2) we also need equality in (80), which can only hold if $\langle f, T_\rho g \rangle = \pm \rho$ by Lemma 5 and part 2 of Lemma 3. Furthermore, $\langle f, T_\rho g \rangle \in \{t_0, t_1\}$ implies equality in either (73) or (77). Together with $\alpha = \beta = 0$, this means by Lemma 4 that $g = \pm f$, which implies $\langle f, T_\rho f \rangle = \rho$. As $\rho \in (0, 1)$ we have by [10, Proposition 2.50] that $f = \pm \chi_i$ for some $i \in [1:n]$.

5. Discussion. The key idea underlying the proof of Theorem 1 is expressed using Fourier-analytic tools in Lemma 4. Based upon this result, we were able to reduce the statement of Theorem 1 to elementary inequalities. It is worth to emphasize that these inequalities—in particular Lemma 9, which contains Lemmas 7 and 8 as special cases—required considerable effort. They might turn out to be useful in the context of other converse proofs concerning the optimization of rate regions with binary random variables.

Although we provided a conclusive and complete proof for the tight upper bound on the mutual information of two Boolean functions, Conjecture 1 remains open. Our proof might provide some insight into the general problem. However, it seems unlikely that the idea behind Lemma 4 can be applied to fully resolve Conjecture 1 affirmatively.

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APPENDIX A: PROOF OF LEMMA 6

The proof of Lemma 6 consists of a series of lemmas, all of which follow from elementary results in real analysis.

A.1. Auxiliary Results.

LEMMA 7. For $x \in (0, 1)$, $y \in [0, 1]$ and $z > 0$,

1. $\psi_1(x, z) := \frac{1}{x^{-z} - 1} + \log(1 - x^z) \geq 0$.
2. $\psi_2(x, y) := 1 - h_0\left(\frac{1+y}{2}\right) - h_0(x) + xh_0(\bar{x}\bar{y}) + \bar{x}h_0(x\bar{y}) \geq 0$,
with equality if and only if either $x = \frac{1}{2}$ or $y = 0$.
3. $\psi_3(y) := 1 - h_0\left(\frac{1}{2} + \frac{y}{1+y}\right) - h_0\left(\frac{y}{1+y}\right) + \frac{1}{1+y}h_0(y) \geq 0$,
with equality if and only if $y \in \{0, 1\}$.

PROOF. To show part 1, fix $z > 0$ and observe that $\lim_{x \downarrow 0} \psi_1(x, z) = 0$. It then suffices to show that $\psi_1(x, z)$ increases in x :

$$(83) \quad \frac{\partial}{\partial x} \psi_1(x, z) = -\frac{1}{(x^{-z} - 1)^2}(-z)x^{-z-1} + \frac{1}{1 - x^z}(-z)x^{z-1}$$

$$(84) \quad = \frac{z}{x(x^{-z} - 1)} \left(\frac{1}{1 - x^z} - 1 \right) \geq 0.$$

Regarding part 2, it is easily verified that $\psi_2(\frac{1}{2}, y) = \psi_2(x, 0) = 0$ for any $y \in [0, 1]$ and $x \in (0, 1)$. Thus, we can assume $x \neq \frac{1}{2}$ in the following. We obtain for $y \in [0, 1]$,

$$(85) \quad \frac{\partial}{\partial y} \psi_2(x, y) = \frac{1}{2} \log_2 \left(\frac{1+y}{1-y} \right) - x\bar{x} \log_2 \left(\frac{y}{x\bar{x}\bar{y}^2} + 1 \right)$$

and

$$(86) \quad \frac{\partial^2}{\partial y^2} \psi_2(x, y) = \frac{y(1-2x)^2}{\log(2)(x+y\bar{x})(1-x\bar{y})(1-y^2)}.$$

Clearly, $\frac{\partial^2}{\partial y^2} \psi_2(x, y) > 0$ for $y \in (0, 1)$ as every factor occurring in (86) is positive. By inspection of (85), $\frac{\partial}{\partial y} \psi_2(x, 0) = 0$. We apply part 1 of Lemma 3 to intervals $[0, 1 - \varepsilon]$ for arbitrarily small $\varepsilon > 0$ and have $0 = \psi_2(x, 0) < \psi_2(x, y)$ for all $y \in (0, 1)$. For $y = 1$, we have $\psi_2(x, 1) = 1 - h_0(x) > 0$.

To prove part 3, note that $\psi_3(0) = \psi_3(1) = 0$ and

$$(87) \quad \psi'_3(y) = \frac{1}{(1+y)^2} \log_2((1+3y)(1-y))$$

for $y \in [0, 1)$. If $\psi_3(y) \leq 0$ for any $y \in (0, 1)$ then f necessarily attains its minimum on $(0, 1)$ and there exists $y^* \in (0, 1)$ with $\psi_3(y^*) \leq 0$ and $\psi'_3(y^*) = 0$ [12, Theorem 5.8]. Clearly $y^* = \frac{2}{3}$ is the only point in $(0, 1)$ with $\psi'_3(y^*) = 0$ and there we have

$$(88) \quad \psi_3\left(\frac{2}{3}\right) = 1 - h_0\left(\frac{1}{2} + \frac{\frac{2}{3}}{1 + \frac{2}{3}}\right) - h_0\left(\frac{\frac{2}{3}}{1 + \frac{2}{3}}\right) + \frac{1}{1 + \frac{2}{3}} h_0\left(\frac{2}{3}\right)$$

$$(89) \quad = \log_2\left(\frac{27}{25}\right) > 0.$$

□

Based on Lemma 7 we show the following two lemmas, which capture the main portion of the proof of Lemma 6.

LEMMA 8. For $0 < a \leq b < 1$,

$$(90) \quad \psi(a, b) := 1 - h_0\left(\frac{1}{2} + \frac{\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}}\right) - h_0(a) + b h_0\left(\frac{a}{b}\right) \geq 0,$$

with equality if and only if $a = b = \frac{1}{2}$.

PROOF. First we consider the case $b = a$ where we have $\psi(a, a) = 1 - h_0(a) \geq 0$, with equality if and only if $b = a = \frac{1}{2}$. Define the open set $J := \{(a, b) \in \mathbb{R}^2 : 0 < a < b < 1\}$. We will show $\psi(a, b) > 0$ for $(a, b) \in J$. To this end, introduce the variable transformation

$$(91) \quad (a, b) \mapsto (x, y) := \left(\sqrt{\frac{ab}{ab}}, \frac{a}{b}\right),$$

and its inverse for $(a, b) \in J$,

$$(92) \quad (x, y) \mapsto (a, b) := \left(\frac{y - x^2}{1 - x^2}, \frac{y - x^2}{y - x^2 y}\right).$$

Also note that $y \in (0, 1)$ and

$$(93) \quad 0 < x^2 = \frac{a\bar{b}}{ab} = y \frac{\bar{b}}{a} < y,$$

thus $(x^2, y) \in J$. We introduce the additional transformation $c := \frac{\log(y)}{2\log(x)}$, yielding $y = x^{2c}$ and

$$(94) \quad 0 < c = \frac{\log(y)}{2\log(x)} < \frac{\log(x^2)}{2\log(x)} = 1,$$

i.e., $(x, c) \in (0, 1)^2$. Now we redefine $\psi(a, b)$ in terms of x and c as

$$(95) \quad \tilde{\psi}(x, c) = 1 - h_0\left(\frac{1}{2} + \frac{x}{1+x}\right) - h_0\left(\frac{x^{2c} - x^2}{1 - x^2}\right) + \frac{1 - x^{2-2c}}{1 - x^2} h_0(x^{2c}).$$

Fix a particular $x \in (0, 1)$ and define $\gamma_x(c) := \tilde{\psi}(x, c)$ for $c \in (0, 1)$. We obtain

$$(96) \quad \gamma'_x(c) = \frac{2 \log(x)}{(x^2 - 1) \log(2)} (2x^{2c} c \log(x) + x^{2(1-c)} \log(1 - x^{2c}) - x^{2c} \log(x^{2c} - x^2)),$$

where clearly $\gamma'_x(\frac{1}{2}) = 0$. The second-order derivative is

$$(97) \quad \gamma''_x(c) = \frac{4 \log(x)^2 x^{2c}}{(1 - x^2) \log(2)} \tilde{\gamma}_x(c)$$

with

$$(98) \quad \begin{aligned} \tilde{\gamma}_x(c) &:= \log(x^{2c} - x^2) - 2c \log(x) + \frac{x^2}{x^{4c}} \log(1 - x^{2c}) \\ &\quad + \frac{x^2}{x^{2c} - x^2} + \frac{x^2}{(1 - x^{2c})x^{2c}} \end{aligned}$$

$$(99) \quad \begin{aligned} &= \log(1 - x^{2(1-c)}) + \frac{x^2}{x^{4c}} \log(1 - x^{2c}) \\ &\quad + \frac{x^2}{x^{2c} - x^2} + \frac{x^2}{(1 - x^{2c})x^{2c}} \end{aligned}$$

$$(100) \quad \begin{aligned} &= \left(\frac{1}{x^{-2(1-c)} - 1} + \log(1 - x^{2(1-c)}) \right) \\ &\quad + \frac{x^2}{x^{4c}} \left(\log(1 - x^{2c}) + \frac{1}{x^{-2c} - 1} \right) \end{aligned}$$

$$(101) \quad \geq 0$$

where the inequality in (101) follows by applying part 1 of Lemma 7 to each term in (100). Since $\tilde{\gamma}_x$ determines the sign of γ''_x , we have $\gamma''_x(c) \geq 0$ for $c \in (0, 1)$. Choose $0 < \varepsilon < 1$ and apply part 1 of Lemma 3 to γ_x with $I = [\varepsilon, 1 - \varepsilon]$. This entails $\gamma_x(c) \geq \gamma_x(\frac{1}{2})$ for $c \in (0, 1)$ as we already established $\gamma'_x(\frac{1}{2}) = 0$ and ε was arbitrary. We conclude the proof by remarking that part 3 of Lemma 7 implies $\gamma_x(\frac{1}{2}) = \tilde{\psi}(x, \frac{1}{2}) > 0$ for $x \in (0, 1)$. \square

LEMMA 9. For $0 < a \leq b < 1$ and $0 \leq \rho \leq \frac{2\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}}$,

$$(102) \quad 0 \leq 1 - h_0\left(\frac{1+\rho}{2}\right) - h_0(a) + bh_0\left(a + \rho \frac{a\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2b}\right) + \bar{b}h_0\left(a - \rho \frac{a\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2\bar{b}}\right),$$

with equality if and only if either $a = b = \frac{1}{2}$ or $\rho = 0$.

PROOF. Fix $0 < a \leq b < 1$ and define

$$(103) \quad A := \frac{a\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2}, \quad \rho_0 := \frac{\min\{ab, \bar{a}\bar{b}\}}{A},$$

$$(104) \quad \rho_1 := \frac{2\sqrt{ab}}{\sqrt{ab} + \sqrt{\bar{a}\bar{b}}} = \frac{a\bar{b}}{A}, \quad \rho_{-1} := \frac{\max\{ab, \bar{a}\bar{b}\}}{A}.$$

We can write (102) as $\phi(\rho) \geq 0$ for $\rho \in [0, \rho_1]$ with

$$(105) \quad \phi(\rho) := 1 - h_0\left(\frac{1+\rho}{2}\right) - h_0(a) + bh_0\left(a + \rho \frac{A}{b}\right) + \bar{b}h_0\left(a - \rho \frac{A}{\bar{b}}\right).$$

Since $\phi(0) = 0$, we can assume $\rho \in (0, \rho_1]$ in the following. Next, consider the case $b = a$. We then have $A = a\bar{a}$ and

$$(106) \quad \phi(\rho) = 1 - h_0\left(\frac{1+\rho}{2}\right) - h_0(a) + ah_0\left(a + \rho \frac{a\bar{a}}{a}\right) + \bar{a}h_0\left(a - \rho \frac{a\bar{a}}{\bar{a}}\right)$$

$$(107) \quad = 1 - h_0\left(\frac{1+\rho}{2}\right) - h_0(a) + ah_0(\bar{a}\bar{\rho}) + \bar{a}h_0(a\bar{\rho})$$

$$(108) \quad \geq 0,$$

by part 2 of Lemma 7, with equality if and only if $a = \frac{1}{2}$.

Assuming $0 < a < b < 1$, we will now show $\phi(\rho) > 0$ for $\rho \in (0, \rho_1]$. We have

$$(109) \quad \phi'(\rho) = \frac{1}{2} \log_2 \left(\frac{1+\rho}{1-\rho} \right) + A \log_2 \left(\frac{(\bar{a}b - A\rho)(a\bar{b} - A\rho)}{(ab + A\rho)(\bar{a}\bar{b} + A\rho)} \right)$$

and

$$(110) \quad \phi''(\rho) = \frac{A^2}{\log 2} \left(\frac{1}{A^2(1-\rho^2)} - \frac{1}{\bar{a}b - A\rho} - \frac{1}{ab - A\rho} - \frac{1}{\bar{a}\bar{b} + A\rho} - \frac{1}{ab + A\rho} \right).$$

Note, that $\phi'(\rho_1)$ and $\phi''(\rho_1)$ are undefined, but

$$(111) \quad \lim_{\rho \uparrow \rho_1} \phi'(\rho) = \lim_{\rho \uparrow \rho_1} \phi''(\rho) = -\infty.$$

Moreover, we have

$$(112) \quad \phi''(0) = \frac{A^2}{\log 2} \left(\frac{1}{A^2} - \frac{1}{\bar{a}b} - \frac{1}{a\bar{b}} - \frac{1}{\bar{a}\bar{b}} - \frac{1}{ab} \right)$$

$$(113) \quad = \frac{1}{\log 2} \left(1 - \frac{A^2}{a\bar{a}b\bar{b}} \right)$$

$$(114) \quad = \frac{1}{\log 2} \left(1 - \left(\frac{\sqrt{a\bar{b}} + \sqrt{\bar{a}b}}{\sqrt{\bar{a}b} + \sqrt{a\bar{b}}} \right)^2 \right)$$

$$(115) \quad > 0$$

as $\bar{a}b < \bar{a}b$. We can write $\phi''(\rho) = \frac{p(\rho)}{q(\rho)}$, where both p and q are polynomials in ρ . We choose

$$(116) \quad q(\rho) = \log(2)(1 - \rho^2)(\bar{a}b - A\rho)(a\bar{b} - A\rho)(\bar{a}\bar{b} + A\rho)(ab + A\rho)$$

and notice that

$$(117) \quad q(\rho) > 0 \quad \text{for } \rho \in [0, \rho_1).$$

And from (110),

$$(118) \quad \begin{aligned} p(\rho) = & (\bar{a}b - A\rho)(a\bar{b} - A\rho)(\bar{a}\bar{b} + A\rho)(ab + A\rho) \\ & - A^2(1 - \rho^2) \left((a\bar{b} - A\rho)(\bar{a}\bar{b} + A\rho)(ab + A\rho) \right. \\ & + (\bar{a}b - A\rho)(\bar{a}\bar{b} + A\rho)(ab + A\rho) \\ & + (\bar{a}b - A\rho)(a\bar{b} - A\rho)(ab + A\rho) \\ & \left. + (\bar{a}b - A\rho)(a\bar{b} - A\rho)(\bar{a}\bar{b} + A\rho) \right). \end{aligned}$$

This entails $\deg(p) \leq 5$, i.e., $p(\rho) = c_5\rho^5 + c_4\rho^4 + c_3\rho^3 + c_2\rho^2 + c_1\rho + c_0$. Calculation of the coefficients reveals $c_5 = c_4 = 0$, implying $\deg(p) \leq 3$.

We will now demonstrate that there is a unique point $\rho^* \in (0, \rho_1)$ with $p(\rho^*) = 0$. To this end, reinterpret $\phi''(\rho)$ as a rational function in ρ on \mathbb{R} . By (111), (115) and (117), we know that the number of zeros of p in $(0, \rho_1)$ is odd and at most equal to its degree, i.e., either one or three. We next show that p has at least one zero in $(-\infty, 0)$, ensuring that there is only one zero in $(0, \rho_1)$. Depending on ρ_0 (cf. (103)), we distinguish four cases:

1. $\rho_0 < 1$: We have $q(\rho) > 0$ for $\rho \in (-\rho_0, 0)$, $\phi''(0) > 0$ and $\lim_{\rho \downarrow -\rho_0} \phi''(\rho) = -\infty$. Thus, there is an odd number of zeros in $(-\rho_0, 0)$.
2. $\rho_0 = 1$: Note that $p(-1) = 0$.
3. $\rho_0 = \rho_{-1}$: Observe that $p(-\rho_0) = 0$.
4. $\rho_{-1} > \rho_0 > 1$: Let $I := (-\rho_{-1}, -\rho_0)$ and observe that $q(\rho) > 0$ for $\rho \in I$. Thus, there needs to be an odd number of zeros in I as $\lim_{\rho \downarrow -\rho_{-1}} \phi''(\rho) = -\infty$ and $\lim_{\rho \uparrow -\rho_0} \phi''(\rho) = \infty$.

Figures 1a and 1b qualitatively illustrate the behavior of $p(\rho)$ and $\phi''(\rho)$ for cases 1 and 4, respectively.

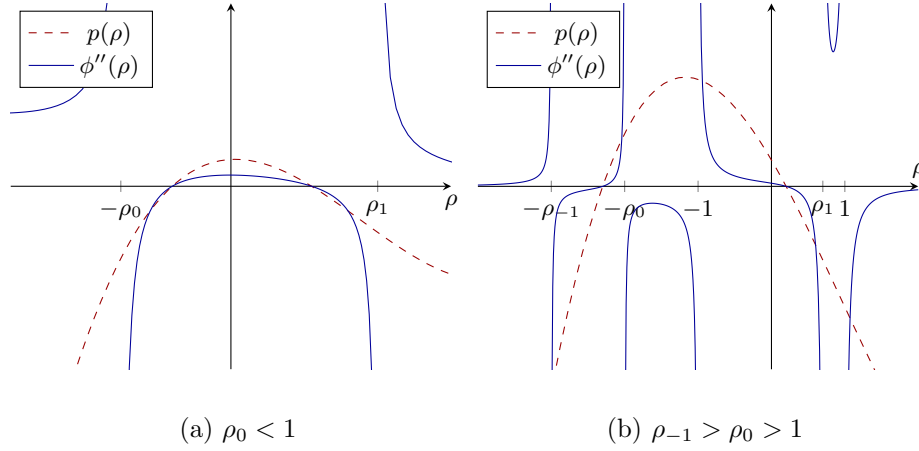


Fig 1: Sketch of $p(\rho)$ and $\phi''(\rho)$.

Consequently $\phi''(\rho) > 0$ for $\rho \in (0, \rho^*)$ and by inspection of (109) we have $\phi'(0) = 0$. Thus, by part 1 of Lemma 3, $\phi(\rho) > \phi(0) = 0$ for $\rho \in (0, \rho^*]$. In particular, $\phi(\rho^*) > 0$. Choose any $\varepsilon \in (0, \rho_1 - \rho^*)$. Since $\phi''(\rho) < 0$ for $\rho \in (\rho^*, \rho_1)$ we have $\phi(\rho) > \min\{\phi(\rho^*), \phi(\rho_1 - \varepsilon)\}$ for all $\rho \in (\rho^*, \rho_1 - \varepsilon)$, by part 2 of Lemma 3. Using (111) and the mean value theorem [12, Theorem 5.10], it follows that $\phi(\rho_1 - \varepsilon) \geq \phi(\rho_1)$ for all $\varepsilon \in (0, \varepsilon_0)$ for some suitably small $\varepsilon_0 > 0$. This implies that $\phi(\rho) > \min\{\phi(\rho^*), \phi(\rho_1)\}$ for $\rho \in (\rho^*, \rho_1)$ as ε was arbitrary. In summary, we have $\phi(\rho) > \min\{0, \phi(\rho_1)\}$ for $\rho \in (0, \rho_1)$ and finish the proof by remarking that $\phi(\rho_1) \geq 0$ was shown in Lemma 8. \square

A.2. Proof of Lemma 6. We will show (54) and (55) by distinguishing four cases. Starting with (54), first assume

$$(119) \quad 1 - 2(\bar{a} + \bar{b}) \geq 1 - 2 \left(a\bar{b} + b\bar{a} + \rho \left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}} \right) \right),$$

which is equivalent to

$$(120) \quad \rho \geq \frac{2\sqrt{\bar{a}\bar{b}}}{\sqrt{\bar{a}\bar{b}} + \sqrt{ab}}.$$

Now $t_0 = 1 - 2(\bar{a} + \bar{b})$ by (52) and

$$(121) \quad 1 - h_0(r) - h_0(a) + \phi_{a,b}(t_0)$$

$$(122) \quad = 1 - h_0(r) - h_0(a) + \phi_{a,b}(1 - 2(\bar{a} + \bar{b}))$$

$$(123) \quad = 1 - h_0(r) - h_0(a) + bh_0\left(\frac{\bar{a}}{b}\right)$$

$$(124) \quad \geq 1 - h_0\left(\frac{1}{2} + \frac{\sqrt{\bar{a}\bar{b}}}{\sqrt{\bar{a}\bar{b}} + \sqrt{ab}}\right) - h_0(a) + bh_0\left(\frac{\bar{a}}{b}\right)$$

$$(125) \quad \geq 0,$$

where (124) follows from (120) and the monotonicity of $h_0(\cdot)$ on $[\frac{1}{2}, 1]$, and (125) follows from Lemma 8 using the substitution $a \mapsto \bar{a}$. Note that equality holds in (125) if and only if $a = b = \frac{1}{2}$, which implies $\rho = 1$, in turn implying equality in (124).

Conversely, for $\rho < \frac{2\sqrt{\bar{a}\bar{b}}}{\sqrt{\bar{a}\bar{b}} + \sqrt{ab}}$, we have $t_0 = 1 - 2\left(\bar{a}\bar{b} + b\bar{a} + \rho\left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right)\right)$ by (52) and obtain

$$(126) \quad \begin{aligned} 1 - h_0(r) - h_0(a) + \phi_{a,b}(t_0) \\ = 1 - h_0(r) - h_0(a) \\ + \phi_{a,b}\left(1 - 2\left(\bar{a}\bar{b} + b\bar{a} + \rho\left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right)\right)\right) \end{aligned}$$

$$(127) \quad \begin{aligned} = 1 - h_0(r) - h_0(a) + bh_0\left(a - \rho\frac{\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2b}\right) \\ + \bar{b}h_0\left(a + \rho\frac{\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}}{2\bar{b}}\right) \end{aligned}$$

$$(128) \quad \geq 0,$$

where (128) follows from Lemma 9 with the substitution $a \mapsto \bar{a}$. Note that equality holds in (128) if and only if either $\rho = 0$ or $a = b = \frac{1}{2}$. This finishes the proof of (54).

To show (55), we first assume

$$(129) \quad 1 + \alpha - \beta \leq 1 - 2\left(\bar{a}\bar{b} + b\bar{a} - \rho\left(\bar{a}\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right)\right),$$

which is equivalent to

$$(130) \quad \rho \geq \frac{2\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}}$$

and implies $t_1 = 1 - 2(b - a)$ by (53). We obtain

$$(131) \quad \begin{aligned} 1 - h_0(r) - h_0(a) + \phi_{a,b}(t_1) \\ = 1 - h_0(r) - h_0(a) + bh_0\left(\frac{a}{b}\right) \end{aligned}$$

$$(132) \quad \geq 1 - h_0\left(\frac{1}{2} + \frac{\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}}\right) - h_0(a) + bh_0\left(\frac{a}{b}\right)$$

$$(133) \quad \geq 0,$$

where (132) holds by (130) and the monotonicity of $h_0(\cdot)$ on $[\frac{1}{2}, 1]$, and (133) is a consequence of Lemma 8. Note that equality holds in (133) if and only if $a = b = \frac{1}{2}$, which implies $\rho = 1$, in turn implying equality in (132).

Conversely, $\rho < \frac{2\sqrt{ab}}{\sqrt{ab} + \sqrt{ab}}$ entails $t_1 = 1 - 2\left(a\bar{b} + b\bar{a} - \rho\left(a\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right)\right)$ by (53) and we obtain

$$(134) \quad 1 - h_0(r) - h_0(a) + \phi_{a,b}(t_1)$$

$$(135) \quad \begin{aligned} = 1 - h_0(r) - h_0(a) + bh_0\left(a + \frac{\rho}{2b}\left(a\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right)\right) \\ + \bar{b}h_0\left(a - \frac{\rho}{2b}\left(a\bar{b} + \sqrt{a\bar{a}b\bar{b}}\right)\right) \end{aligned}$$

$$(136) \quad \geq 0,$$

where (136) follows from Lemma 9. Note that equality holds in (136) if and only if either $\rho = 0$ or $a = b = \frac{1}{2}$.

REFERENCES

- [1] AHLWEDE, R. and GACS, P. (1976). Spreading of sets in product spaces and hypercontraction of the Markov operator. *Ann. of Probability* **4** 925–939.
- [2] ANANTHARAM, V., GOHARI, A. A., KAMATH, S. and NAIR, C. (2013). On hypercontractivity and the mutual information between Boolean functions. In *Proc. 51st Allerton Conf. Commun., Control, Comput.* 13–19.
- [3] COURTADE, T. A. and KUMAR, G. R. (2014). Which Boolean functions maximize mutual information on noisy inputs? *IEEE Trans. Inf. Theory* **60** 4515–4525.
- [4] COVER, T. M. and THOMAS, J. A. (2006). *Elements of Information Theory*. Wiley-Interscience.
- [5] GARBAN, C. and STEIF, J. E. (2014). *Noise Sensitivity of Boolean Functions and Percolation* **5**. Cambridge University Press.

- [6] KAHN, J., KALAI, G. and LINIAL, N. (1988). The influence of variables on Boolean functions. In *Proc. 29th Annual Symposium on Foundations of Computer Science* 68–80. IEEE.
- [7] KINDLER, G., O’DONNELL, R. and WITMER, D. (2016). Remarks on the most informative function conjecture at fixed mean. *preprint*. [arXiv:1506.03167](https://arxiv.org/abs/1506.03167)
- [8] KLOTZ, J. G., KRACHT, D., BOSSERT, M. and SCHÖBER, S. (2014). Canalizing Boolean functions maximize mutual information. *IEEE Trans. Inf. Theory* **60** 2139–2147.
- [9] KUMAR, G. R. and COURTADE, T. A. (2013). Which Boolean functions are most informative? In *Proc. IEEE Int. Symp. on Inform. Theory* 226–230.
- [10] O’DONNELL, R. (2014). *Analysis of Boolean Functions*. Cambridge University Press.
- [11] ORDENTLICH, O., SHAYEVITZ, O. and WEINSTEIN, O. (2015). An improved upper bound for the most informative Boolean function conjecture. *preprint*. [arXiv:1505.05794](https://arxiv.org/abs/1505.05794)
- [12] RUDIN, W. (1976). *Principles of Mathematical Analysis*, 3rd ed. McGraw-Hill.
- [13] RUDIN, W. (1987). *Real and Complex Analysis*, 3rd ed. McGraw-Hill.
- [14] TALAGRAND, M. (1993). Isoperimetry, logarithmic Sobolev inequalities on the discrete cube, and Margulis’ graph connectivity theorem. *Geometric & Functional Analysis* **3** 295–314.
- [15] TALAGRAND, M. (1994). On Russo’s approximate zero-one law. *Ann. of Probability* 1576–1587.

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